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Spectral studies of some (5-substituted phenyl) isoxazole based sydnones: Assessment of substituent effects

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ABSTRACT

About ten 4-(N-(4-(5-phenylisoxazol-3-yl)phenylsufamyl)-3-(p-tolyl)-1,2,3,-oxadiazol-3-ium-5-olates were synthesised and examined their purities by literature method. The infrared and NMR spectral data of above synthesised isoxazoles were assigned and correlated with Hammett substituent constants and Swain-Lupton's constants using regression analysis. From statistical analyses results, the effects of substituents on the spectral data have been discussed.

***Keywords*:** Sydnone isoxazole; IR spectra; NMR spectra; Spectral LFER; Hammett substituent constants

1. INTRODUCTION

Isoxazoles are five membered heterocyclic compounds containing N and O atoms neighbouring positions [1]. They possess many biological and medicinal properties [2-5]. These isoxazoles were prepared by cyclisation of chalcones with hydroxylamine under

solvent assisted and solvent-free conditions [5,6]. The five membered mesoionic dipolar compounds are known as sydnones [7]. From other aromatics, they are fairly difference compounds with reactivity and stability [8]. They are important compounds in medicinal, heterocyclic and theoretical chemistry [9].

These sydnones were used as key intermediates for synthesis of organic compounds and possess physiological potentials. They possess many biological activities such as antimicrobial [10], antiviral [11], anti-tumour [12], analgesic [13], anti-inflammatory [14], anthelmintic [15], free-radical scavenging [16], nitric oxide donor [17] and anti-cancer [18]. Spectroscopic data were useful for prediction of geometry and ground state equilibration of organic compounds [19]. From vibrational spectra the *s-cis* and *s-trans* conformations of carbonyl compounds were predicted [20]. The chemical shifts of NMR spectra were useful for prediction of geometry of compounds such as *E* or *Z* along with coupling constants [21].

Proton chemical shifts splitting patterns used for prediction of spatial arrangement of heterocyclic ring protons in cyclohexane and five membered pyrazolines [22]. Correlation analysis was used for studying reaction speeds, structural conformations of alkenes [23], alkynes [24], α,β- unsaturated aldehydes [25], ketones [26], ω-substituted ketones [27] and its esters, halo acyl bromides [28], ^{1}H pyrazoles [29] and its derivatives. Thirunarayanan and Manikandan have studied the dosage of drug analysis using correlation study [30]. Thirunarayanan et al., have studied the infrared and NMR spectral correlations of phenazine and quinoxaline derivatives [27,28].

Mayavel et al., have studied the spectral correlation of some *E*-imines [29]. The Qsar and Qpr spectral correlation of some dihyroisoxazoles were reported by Thirunarayanan et al., [31]. Thirunarayanan and his co-workers have studied the effect of substituents on spectral data of some isoxazole-2-amines [32].

The spectral correlation of infrared and carbon-13 NMR data of quinoxaline and phenazine derivatives were studied by Thirunaryanan et al. [33,34]. Senbagam et al., have studied the effects of substituents on some substituted (*E*)-*N*-benzylidene-4*H*-1,2,4-triazol-4-amines [35]. Vijayakumar et al., have investigated the spectral correlation analysis on some (*E*)-2-benzylidenehydrazine carbothioamides [36].

The effect of substituents on some hydrazine derivatives were investigated by Rajarajan et al., [37]. On the complete literature survey, the similar study was not reported with isoxazole based sydnones. Hence, the authors have reported first time to the study of spectral correlation of the titled compounds by IR and NMR spectra.

2. EXPERIMENTAL

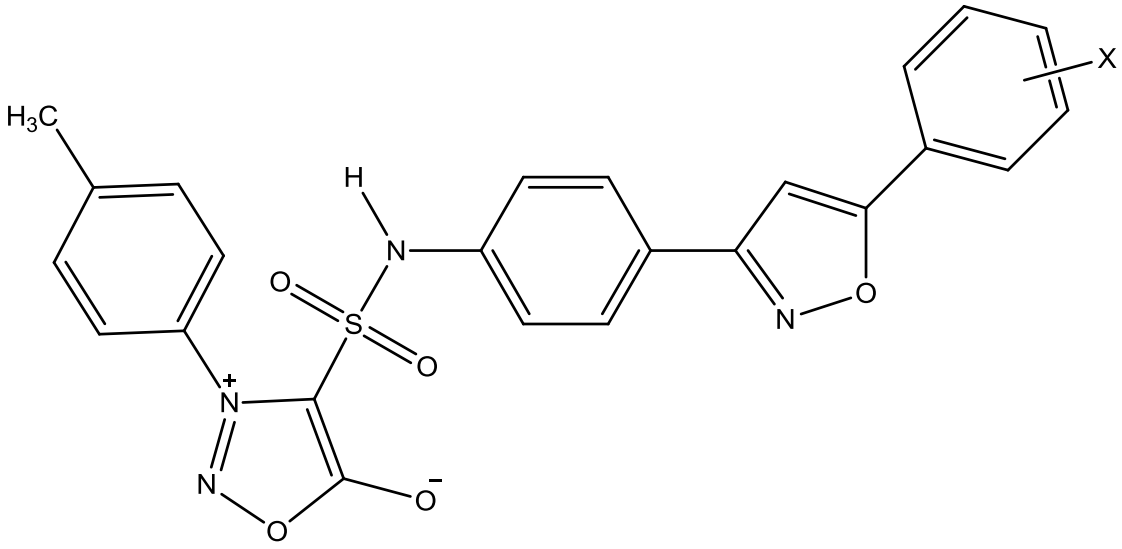
2. 1. General

In this present investigations, chemicals used were purchased from Sigma-Aldrich Company Bangalore, India. Infrared spectra (KBr, 4000-400 cm^{-1}) were recorded on a Briker (Thermo Nicolet) Fourier transform spectrophotometer.

The NMR spectra of all pyrazolines were recorded on a Bruker AV400 spectrometer operating at 400 MHz to record 1 H and 100 MHz for 13C spectra in $CDCl_3$ solvent with TMS as internal standard.

2. 2. Synthesis of 4-(N-(4-(5-phenylisoxazol-3-yl)phenylsufamyl)-3-(p-tolyl)-1,2,3,-oxadiazol-3-ium-5-olates

In this present study, the titled compounds were synthesised and characterized by literature method [38]. The general structure of 4-(N-(4-(5-phenylisoxazol-3-yl) phenylsufamyl)-3-(p-tolyl)-1,2,3,-oxadiazol-3-ium-5-olates are shown in Fig. 1.



X= H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2

Fig. 1. The general structure of 4-(N-(4-(5-phenylisoxazol-3-yl)phenylsufamyl)-3-(p-tolyl)-1,2,3,-oxadiazol-3-ium-5-olates.

3. RESULTS AND DISCUSSION

3. 1. Correlation analysis of IR spectral data

Infrared spectra of synthesized 4-(N-(4-(5-phenylisoxazol-3-yl)phenylsufamyl)-3-(p-tolyl)-1,2,3,-oxadiazol-3-ium-5-olates, the characteristic stretches (ν, cm^{-1}) of $CN(C_3)$, NH, SO_2, and CO_{syd} have been assigned and tabulated in Table 1. Using Hammett equation and single and multi-regression analysis [19-22,26-37] of these data with Hammett substituent constants and Swain-Lupton's [39] parameters. In this correlation, the Hammett equation was taken in the form as (1).

Table 1. The infrared characteristics vibrations (ν, cm^{-1}) of 4-(N-(4-(5-phenylisoxazol-3-yl) phenylsufamyl)-3-(p-tolyl)-1,2,3,-oxadiazol-3-ium-5-olates.

Entry	X	CN	NH	SO_2	CO_{syd}
1	H	1649	3382	1319	1755
2	3-Br	1655	3386	1326	1758

3	2-Cl	1654	3383	1327	1757
4	4-Cl	1658	3384	1325	1756
5	4-F	1653	3386	1326	1758
6	4-OH	1656	3385	1328	1756
7	2-OCH_3	1646	3377	1320	1748
8	4-OCH_3	1645	3378	1316	1751
9	4-CH_3	1652	3380	1322	1753
10	4-NO_2	1663	3394	1332	1761

$$\nu = \nu_o + \rho\sigma \qquad \ldots(1)$$

where:
ν_o is the unsubstitued system.

The obtained statistical results are tabulated in Table 2. From the Table 2, the CN stretches (ν, cm^{-1}) gave satisfactory correlations with Hammett substituent constants and F parameters along with positive ρ values. This ρ value indicates that, the normal substituent effects operate in all systems. The R parameter was fail in correlation. The failure in correlation was the inability of prediction of effects of substituents on the stretches and attributed with the resonance-conjugative structure as illustrated in Fig. 2.

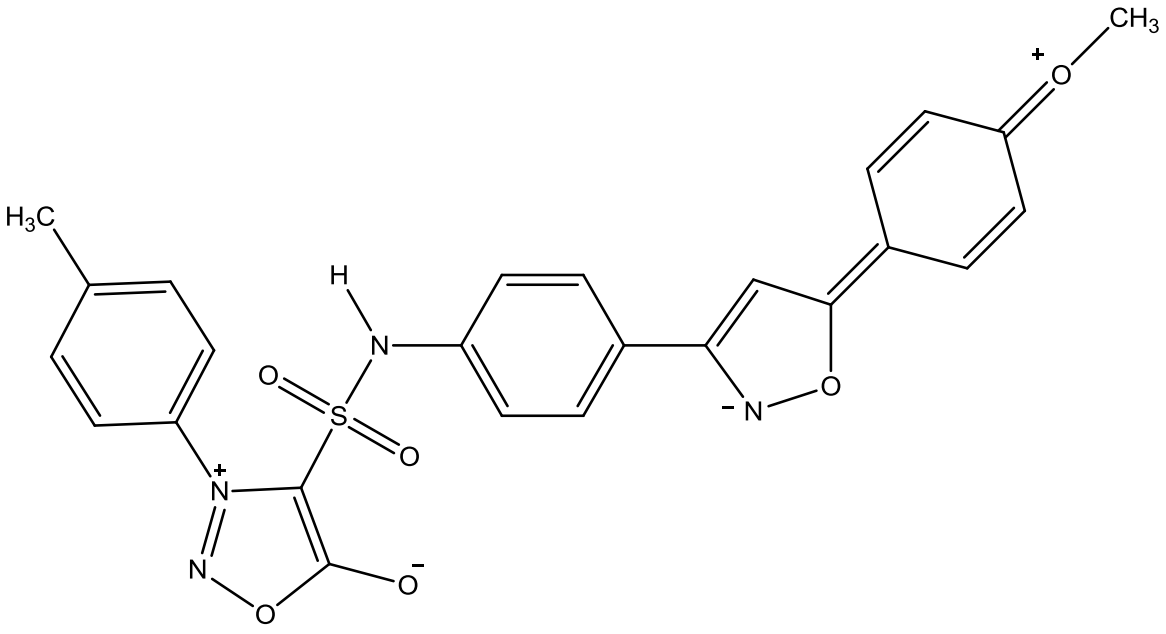


Fig. 2. The resonance-conjugative structure.

Table 2. Results of statistical analysis of infrared vibrations (ν, cm^{-1}) of 4-(N-(4-(5-phenylisoxazol-3-yl)phenylsufamyl)-3-(p-tolyl)-1,2,3,-oxadiazol-3-ium-5-olates with Hammett σ, σ^+, σ_I, σ_R constants, F and R parameters.

Frequency	Constant	r	I	ρ	s	n	Correlated derivatives
CN	σ	0.976	1652.58	11.316	3.71	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ^+	0.962	1653.61	6.231	4.32	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_I	0.905	1648.29	14.785	4.70	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_R	0.905	1656.41	13.411	4.75	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	F	0.905	1648.71	12.482	4.91	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	R	0.814	1655.99	9.288	5.10	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
NH	σ	0.983	3382.99	10.966	2.82	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ^+	0.966	3388.97	5.897	3.83	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_I	0.965	3378.87	14.165	3.89	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_R	0.957	3386.47	12.040	4.20	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	F	0.965	3378.68	13.383	3.90	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	R	0.846	3386.02	8.088	4.56	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
SO_2	σ	0.966	1323.70	8.648	3.78	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2

	σ^+	0.957	1324.50	5.003	4.16	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_I	0.967	1319.23	14.376	3.75	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_R	0.834	1325.83	7.008	4.71	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	F	0.965	1319.32	13.264	3.83	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	R	0.823	1325.49	4.564	4.91	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
CO_{syd}	σ	0.982	1754.91	8.413	2.24	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ^+	0.978	1755.99	4.823	2.84	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_I	0.958	1751.95	9.837	3.24	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_R	0.958	1757.65	9.504	3.23	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	F	0.959	1751.91	9.417	3.22	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	R	0.846	1757.27	6.348	3.53	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
r = correlation coefficient; ρ = slope; I = intercept; s = standard deviation; n = number of substituents							

The NH stretches (ν, cm^{-1}) of isoxazole sydnones gave satisfactory correlation with Hammett substituent constants and F parameters. Here also the R parameter was fail producing satisfactory correlation.

The satisfactory correlations obtained for the SO_2 stretches (ν, cm^{-1}) of sydnones with Hammett σ, σ+, σ_I constants and F parameters. The resonance components were fail for giving good correlation coefficients. A satisfactory correlation was obtained for CO_{syd} (ν, cm^{-1}) of sydnones with Hammett substituent constants and F parameters. Here also the R parameter was fail producing satisfactory correlation. The reason for failure in correlation was already stated and along with resonance-conjugation structure as illustrated in Fig. 2.

In single parameter infrared spectral correlations, some of the Hammett substituent constants, F and R parameters were fail for giving correlation coefficients. When these data are produced satisfactory correlations in multi-regression analysis with σ_I, σ_R and Swain-Lupton's constants [39]. The generated multi-regression analysis equations are given in (2-9).

$$\nu CN(cm^{-1}) = 1651.61\ (\pm 2.463) + 14.976(\pm 5.258)\sigma_I + 13.410(\pm 5.094)\sigma_R \quad \ldots(2)$$
(R = 0.981, n=10, P > 95%)

$$\nu CN(cm^{-1}) = 1651.51(\pm 2.721) + 13.762(\pm 5.720)F + 10.728(\pm 4.871)R \quad \ldots(3)$$
(R = 0.975, n=10, P > 95%)

$$\nu NH(cm^{-1}) = 3381.67(\pm 1.844) + 14.645(\pm 3.985)\sigma_I + 12.040(\pm 3.815)\sigma_R \quad \ldots(4)$$
(R = 0.987, n=10, P > 95%)

$$\nu NH(cm^{-1}) = 3381.18(\pm 1.940) + 14.769(\pm 4.077)F + 9.633(\pm 3.477)R \quad \ldots(5)$$
(R = 0.985, n=10, P > 95%)

$$\nu SO(cm^{-1}) = 1320.96(\pm 2.465) + 14.375(\pm 5.271)\sigma_I + 7.007(\pm 5.081)\sigma_R \quad \ldots(6)$$
(R = 0.975, n=10, P > 90%)

$$\nu SO(cm^{-1}) = 1320.87(\pm 2.462) + 14.120(\pm 5.717)F + 5.942(\pm 2.144)R \quad \ldots(7)$$
(R = 0.974, n=10, P > 90%)

$$\nu CO_{syd}(cm^{-1}) = 1754.31(\pm 1.644) + 9.843(\pm 3.524)\sigma_I + 9.503(\pm 3.340)\sigma_R \quad \ldots(8)$$
(R = 0.983, n=10, P > 95%)

$$\nu CO_{syd}(cm^{-1}) = 1753.84(\pm 1.710) + 10.487(\pm 3.595)F + 7.445(\pm 3.065)R \quad \ldots(9)$$
(R = 0.980, n=10, P > 90%)

3. 2. NMR Spectral correlations

3. 2. 1. ^{1}H NMR spectral study

In the present correlation analysis study, the compounds chosen for evaluating the effects of substituents on the sydnone isoxazoles were shown in Fig. 1. The NMR spectra of synthesised sydnone isoxazoles were recorded in $CDCl_3$ solvent using TMS as internal standard. The chemical shifts (δ, ppm) of isoxazole ring proton H_4, NH and methyl protons of synthesised sydnone isoxazoles were presented in Table 3. These chemical shifts(δ, ppm) have been correlated with Hammett substituent constants, F and R parameters using single and multi-linear regression analysis [19-22,26-38]. In this correlation the Hammett equation was taken in the form as (10)

$$\delta = \rho\sigma + \delta_o \quad \ldots(10)$$

where:
δ_o is the frequency for the parent member of the series.

Table 3. The ^{1}H NMR chemical shifts (δ, ppm) of 4-(N-(4-(5-phenylisoxazol-3-yl)phenylsufamyl)-3-(p-tolyl)-1,2,3,-oxadiazol-3-ium-5-olates.

Entry	X	H_{oxa}	NH	CH_3
1	H	6.796	9.631	2.354
2	3-Br	6.881	9.682	2.383
3	2-Cl	6.813	9.644	2.407
4	4-Cl	6.807	9.635	2.413
5	4-F	6.815	9.645	2.414
6	4-OH	6.809	9.638	2.368
7	2-OCH_3	6.783	9.63	2.347
8	4-OCH_3	6.781	9.628	2.346
9	4-CH_3	6.793	9.642	2.349
10	4-NO_2	6.895	9.653	2.437

The results of statistical analysis of these proton chemical shifts of sydnone isoxazoles with Hammett substituent constants were presented in Table 4. From Table 4, the correlation of H_4 chemical shifts (ppm) of sydnone isoxazoles gave satisfactory correlation coefficients with Hammett substituent constants, F and R parameters.

Table 4. Results of statistical analysis of ^{1}H NMR chemical shifts (δ, ppm) of 4-(N-(4-(5-phenylisoxazol-3-yl)phenylsufamyl)-3-(p-tolyl)-1,2,3,-oxadiazol-3-ium-5-olates with Hammett substituent constants, F and R parameters.

Frequency	Constant	r	I	ρ	s	n	Correlated derivatives
H_{oxa}	σ	0.986	6.813	0.091	0.02	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ^+	0.974	6.823	0.052	0.02	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_I	0.964	6.779	0.112	0.03	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_R	0.958	6.843	0.097	0.03	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3,

							4-NO_2
	F	0.954	6.783	0.094	0.03	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	R	0.957	6.839	0.074	0.03	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
NH	σ	0.962	0.964	0.026	0.01	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ^+	0.958	9.641	0.016	0.01	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_I	0.844	9.644	0.030	0.02	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_R	0.831	9.632	0.023	0.03	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	F	0.840	9.648	0.026	0.02	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	R	0.829	9.633	0.016	0.04	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
CH_3	σ	0.981	2.378	0.074	0.02	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ^+	0.974	2.358	0.045	0.02	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_I	0.984	2.339	0.126	0.01	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_R	0.836	2.394	0.052	0.03	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	F	0.981	2.340	0.115	0.02	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	R	0.836	2.395	0.044	0.03	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
r = correlation coefficient; ρ = slope; I = intercept; s = standard deviation; n = number of substituents							

The Hammett σ, σ^+ constants gave satisfactory correlation with the chemical shifts(ppm) of NH protons of the synthesised sydnone isoxazoles. The Hammett σ_I, σ_R constants, F and R parameters gave poor correlations with NH proton chemical shifts(ppm) of sydnone isoxazoles.

The methyl proton chemical shifts (ppm) gave satisfactory correlation with Hammett σ, σ^+ , σ_I constants and F parameters. Here the resonance components were fail in correlation. The reason for failure in correlation was already stated and associated with resonance-conjugative structure as shown in Fig. 2. In proton chemical shift correlations, all single regressions gave positive ρ values. This means that the normal substituent effect operates in all system.

In single parameter proton chemical shift correlations, some of them are failed. While seeking these in multi-regression analysis [39], they are worthwhile and produced satisfactory correlations. The generated multi-regression analysis equations are given in (11-16).

$$\delta H_{oxa}(ppm) = 6.803(\pm0.015) + 0.122(\pm0.032)\sigma_I + 0.0970(\pm0.031)\sigma_R \quad \ldots(11)$$
(R = 0.986, n=10, P > 95%)

$$\delta H_{oxa}(ppm) = 6.804(\pm0.017) + 0.106(\pm0.036)F + 0.083(\pm0.031)R \quad \ldots(12)$$
(R = 0.981, n=10, P > 95%)

$$\delta NH(ppm) = 9.638(\pm0.010) + 0.030(\pm0.021)\sigma_I + 0.023(\pm0.002)\sigma_R \quad \ldots(13)$$
(R = 0.956, n=10, P > 95%)

$$\delta NH(ppm) = 9.638(\pm0.010) + 0.029(\pm0.012)F + 0.019(\pm0.001)R \quad \ldots(14)$$
(R = 0.952, n=10, P > 95%)

$$\delta CH_3(ppm) = 2.352(\pm0.014) + 0.1262(\pm0.022)\sigma_I + 0.052(\pm0.021)\sigma_R \quad \ldots(15)$$
(R = 0.991, n=10, P > 95%)

$$\delta CH_3(ppm) = 2.355(\pm0.008) + 0.123(\pm0.018)F + 0.057(\pm0.015)\ R \quad \ldots(16)$$
(R = 0.994, n=10, P > 95%)

3. 2. 2. ^{13}C NMR spectral study

The ^{13}C NMR spectral CN(C_3), C_4, C_5, Ar-C-C_5, Ar-C-Cn, Ar-C-NH, CS, CO, Ar-C-N^+, Ar-C-CH_3 and CH_3 chemical shifts(ppm) of synthesised sydnone isoxazoles are presented and Table 5. These data are correlated with Hammett substituent constants, F and R parameters using single and multi-linear regression analysis [19-22,26-38].

The results of single parameter correlation analysis of ^{13}C NMR spectral chemical shifts(ppm) of synthesised sydnone isoxazoles are tabulated in Table 6. From Table 6, the correlation of δCN (ppm) of the isoxazoles gave satisfactory correlation coefficients with Hammett σ, σ^+, σ_I constants and F parameters.

The remaining Hammett σ_R constants and R parameters fail in correlations. This is due to the inability of substituents effects already stated and associated with conjugative structure as shown in Fig. 2.

Table 5. The ^{13}C NMR chemical shifts (δ, ppm) of 4-(N-(4-(5-phenylisoxazol-3-yl)phenylsufamyl)-3-(p-tolyl)-1,2,3,-oxadiazol-3-ium-5-olates.

Entry	X	CN(C_3)	C_4	C_5	Ar-C-C_5	Ar-C-C_3	Ar-C-NH
1	H	162.48	101.37	158.35	136.39	118.34	137.63
2	3-Br	162.57	102.37	158.32	136.23	118.12	137.86
3	2-Cl	162.45	102.41	158.41	136.25	118.25	137.81
4	4-Cl	162.53	102.43	158.44	136.32	118.23	137.84
5	4-F	162.52	102.56	158.46	136.33	118.26	137.85
6	4-OH	162.58	101.28	158.45	136.35	118.19	137.64
7	2-OCH_3	162.34	101.24	158.31	136.29	118.22	137.62
8	4-OCH_3	162.28	101.18	158.29	136.24	118.18	137.56
9	4-CH_3	162.36	102.26	158.43	136.37	118.25	137.69
10	4-NO_2	162.66	102.58	158.61	136.44	118.97	137.89
Entry	X	C-S	CO_{syd}	Ar-C-N^+	Ar-C-CH_3	CH_3	C-S
1	H	110.71	174.85	135.72	144.68	22.76	110.71
2	3-Br	110.67	174.68	135.82	144.73	22.78	110.67
3	2-Cl	110.61	174.75	135.76	144.77	23.06	110.61
4	4-Cl	110.46	174.46	135.78	144.69	24.05	110.46
5	4-F	110.42	174.42	135.71	144.62	24.65	110.42
6	4-OH	110.43	174.54	135.66	144.57	24.68	110.43
7	2-OCH_3	110.38	174.55	135.6	144.58	24.58	110.38
8	4-OCH_3	110.36	174.42	135.62	144.52	24.52	110.36
9	4-CH_3	110.39	174.38	135.68	144.65	24.61	110.39
10	4-NO_2	110.87	174.96	135.88	144.82	24.98	110.87

The isoxazole ring C_4 carbon chemical shifts(ppm) of 4-(N-(4-(5-phenylisoxazol-3-yl) phenylsufamyl)-3-(p-tolyl)-1,2,3,-oxadiazol-3-ium-5-olates with Hammett σ, σ^+, σ_I constants and F parameters. The remaining Hammett σ_R constants and R parameters fail in correlations.

The isoxazole C_5 carbon chemical shifts(ppm) of 4-(N-(4-(5-phenylisoxazol-3-yl)phenylsufamyl)-3-(p-tolyl)-1,2,3,-oxadiazol-3-ium-5-olates with Hammett substituent σ constants only gave the satisfactory correlation. The remaining Hammett σ^+, σ_I, σ_R constants, F and R parameters were fail in correlations.A satisfactory correlation coefficients obtained for the correlation of Ar-C-C_5 carbon chemical shifts(ppm) of sydnone isoxazoles with only resonance components. Hammett σ, σ^+, σ_I constants and F parameters were fail in correlations. The correlation of Ar-C-CN carbon chemical shifts(ppm) of sydnone isoxazoles with Hammett substituent constants, F and R parameters fail for producing satisfactory correlation coefficients.

The chemical shifts(ppm) of Ar-C-NH carbons of 4-(N-(4-(5-phenylisoxazol-3-yl)phenylsufamyl)-3-(p-tolyl)-1,2,3,-oxadiazol-3-ium-5-olates with Hammett σ, σ^+, σ_I constants and F parameters produced satisfactory correlation. Here, the resonance components of the substituents were fail for giving satisfactory correlations.The CS carbons chemical shifts(ppm) 4-(N-(4-(5-phenylisoxazol-3-yl)phenylsufamyl)-3-(p-tolyl)-1,2,3,-oxadiazol-3-ium-5-olates with Hammett σ, σ^+, σ_R constants and R parameters produced satisfactory correlation. The remaining Hammett σ_I constants and F parameters were failed for producing satisfactory correlations. The chemical shifts(ppm) of Ar-C-N^+ carbons of 4-(N-(4-(5-phenylisoxazol-3-yl)phenylsufamyl)-3-(p-tolyl)-1,2,3,-oxadiazol-3-ium-5-olates with Hammett σ, σ^+, σ_I, σ_R constants and R parameters produced satisfactory correlation. Here, the Field component of the substituents were fail for producing satisfactory correlations.

The correlation of CO_{syd} carbons chemical shifts(ppm) of 4-(N-(4-(5-phenylisoxazol-3-yl)phenylsufamyl)-3-(p-tolyl)-1,2,3,-oxadiazol-3-ium-5-olates with Hammett σ, σ^+, σ_R constants and R parameters produced satisfactory correlation. Hammett σ_I constant and F parameters were failed for producing satisfactory correlations. The chemical shifts(ppm) of Ar-C-CH_3 carbons of 4-(N-(4-(5-phenylisoxazol-3-yl)phenylsufamyl)-3-(p-tolyl)-1,2,3,-oxadiazol-3-ium-5-olates with Hammett σ, σ^+, σ_R constants and R parameters produced satisfactory correlation. Here, the Hammett σ_I constant and F parameters were fail for producing satisfactory correlations. The correlation of CH_3 carbon chemical shifts(ppm) of 4-(N-(4-(5-phenylisoxazol-3-yl)phenylsufamyl)-3-(p-tolyl)-1,2,3,-oxadiazol-3-ium-5-olates with Hammett substituent constants, F and R parameters produced poor correlation. Already stated reason for the poor correlation and it associated with resonance-conjugative structure as shown in Fig. 2. In carbon-13 NMR data correlation study, all correlations gave positive ρ values. This implies that the normal substituent effects operates in all sytesms.

Table 6. Results of statistical analysis of ^{13}C NMR chemical shifts (δ, ppm) of 4-(N-(4-(5-phenylisoxazol-3-yl)phenylsufamyl)-3-(p-tolyl)-1,2,3,-oxadiazol-3-ium-5-olates with Hammett substituent constants, F and R parameters.

Frequency	Constant	r	I	ρ	s	n	Correlated derivatives
C=N(C_3)	σ	0.970	162.46	0.227	0.10	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ^+	0.956	162.48	0.122	0.10	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2

	σ_I	0.955	162.37	0.297	0.10	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_R	0.848	162.53	0.249	0.11	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	F	0.954	162.37	0.275	0.10	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	R	0.836	162.52	0.175	0.11	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
C_4	σ	0.976	101.91	1.268	0.41	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ^+	0.977	102.03	0.860	0.40	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_I	0.956	101.44	1.531	0.23	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_R	0.845	102.26	1.192	0.57	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	F	0.956	101.44	1.441	0.53	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	R	0.847	102.29	1.033	0.57	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
C_5	σ	0.959	158.41	0.152	0.08	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ^+	0.846	158.41	0.079	0.09	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_I	0.844	158.34	0.189	0.09	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_R	0.848	158.45	0.196	0.08	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	F	0.848	158.33	0.96	0.08	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2

	R	0.837	185.44	0.132	0.09	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
Ar-C-C_5	σ	0.826	134.31	0.048	0.07	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ^+	0.817	134.32	0.022	0.07	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_I	0.814	134.33	0.043	0.07	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_R	0.954	134.36	0.169	0.06	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	F	0.846	134.35	0.115	0.05	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	R	0.956	134.37	0.118	0.06	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
Ar-C-C_3	σ	0.815	119.87	9.150	23.18	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ^+	0.834	121.41	3.889	22.02	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_I	0.820	118.34	0.531	22.91	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_R	0.802	122.33	0.236	23.47	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	F	0.809	122.19	8.638	23.36	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	R	0.810	123.07	8.679	23.32	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
Ar-C-NH	σ	0.985	137.72	0.283	0.06	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ^+	0.983	137.60	0.186	0.07	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2

	σ_I	0.974	137.75	0.408	0.08	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_R	0.842	137.79	0.223	0.11	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	F	0.971	137.60	0.369	0.09	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	R	0.844	137.80	0.195	0.11	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
CS	σ	0.983	110.51	0.930	0.10	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ^+	0.981	110.55	0.251	0.10	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_I	0.831	110.44	0.264	0.17	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_R	0.980	110.67	0.600	0.10	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	F	0.821	110.47	0.157	0.18	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	R	0.980	110.68	0.500	0.11	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
CO_{syd}	σ	0.964	174.58	0.349	0.16	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ^+	967	174.62	0.246	0.15	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_I	0.826	174.52	0.232	0.20	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_R	0.965	174.73	0.559	0.16	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	F	0.811	174.56	0.096	0.21	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2

	R	0.968	174.75	0.492	0.15	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
Ar-C-N^+	σ	0.997	135.71	0.232	0.02	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ^+	0.990	135.73	0.145	0.03	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_I	0.958	135.64	0.228	0.07	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_R	0.977	135.79	0.293	0.05	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	F	0.840	135.66	0.175	0.08	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	R	0.974	135.79	0.238	0.06	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
Ar-C-CH_3	σ	0.993	144.76	0.228	0.04	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ^+	0.995	144.67	0.163	0.02	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_I	0.844	144.65	0.186	0.08	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_R	0.977	144.74	0.313	0.06	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	F	0.830	144.62	0.119	0.09	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	R	0.983	144.75	0.280	0.05	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
CH_3	σ	0.820	24.08	0.478	0.89	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ^+	0.830	24.09	0.598	0.84	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2

	σ_I	0.813	24.88	0.953	0.90	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	σ_R	0.828	24.80	1.053	0.87	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	F	0.827	23.70	0.993	0.87	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
	R	0.836	23.71	1.123	0.85	10	H, 3-Br, 2-Cl, 4-Cl, 4-F, 4-OH, 2-OCH_3, 4-OCH_3, 4-CH_3, 4-NO_2
r = correlation coefficient; ρ = slope; I = intercept; s = standard deviation; n = number of substituents							

In single parameter correlation, some of the carbon chemical shifts of (ppm) 4-(N-(4-(5-phenylisoxazol-3-yl)phenylsufamyl)-3-(p-tolyl)-1,2,3,-oxadiazol-3-ium-5-olates failed for production of good correlation coefficients.

These are worthwhile while seeking in multi-regression analysis with σ_I and σ_R constants and Swain-Lupton's [39] F and R parameters. The generated multi-regression equations are given in (17-38).

$$\delta CN(ppm) = 162.43(\pm0.063) + 0.297(\pm0.136)\sigma_I + 0.247(\pm0.131)\sigma_R \quad \ldots(17)$$
(R = 0.973, n=10, P > 95%)

$$\delta CN(ppm) = 162.42(\pm0.065) + 0.302(\pm0.132)F + 0.189(\pm0.011)R \quad \ldots(18)$$
(R = 0.969, n=10, P > 95%)

$$\delta C_4(ppm) = 101.74(\pm0.329) + 1.531(\pm0.707)\sigma_I + 1.192(\pm0.681)\sigma_R \quad \ldots(19)$$
(R = 0.972, n=10, P > 95%)

$$\delta C_4(ppm) = 101.76(\pm0.290) + 1.620(\pm0.609)F + 1.209(\pm0.520)R \quad \ldots(20)$$
(R = 0.978, n=10, P > 90%)

$$\delta C_5(ppm) = 158.39(\pm0.056) + 0.189(\pm0.120)\sigma_I + 0.196(\pm0.117)\sigma_R \quad \ldots(21)$$
(R = 0.965, n=10, P > 95%)

$$\delta C_5(ppm) = 158.37(\pm0.054) + 0.218(\pm0.113)F + 0.155(\pm0.097)R \quad \ldots(22)$$
(R = 0.966, n=10, P > 95%)

$$\delta Ar\text{-}C\text{-}C_5(ppm) = 134.35(\pm0.046) + 0.002(\pm0.001)\sigma_I + 0.114(\pm0.083)\sigma_R \quad \ldots(23)$$
(R = 0.946, n=10, P > 95%)

$$\delta Ar\text{-}C\text{-}C_5(ppm) = 134.37(\pm0.044) + 0.043(\pm0.003)F + 0.161(\pm0.092)\,R \quad \ldots(24)$$
(R = 0.956, n=10, P > 95%)

δAr-C-C_3(ppm) = 118.39(±16.933) + 20.531(±3.633)σ_I + 0.234(±0.035)σ_R …(25)
(R = 0.920, n=10, P > 90%)

δAr-C-C_3(ppm) =124.71(±16.694) + 10.038(±3.508)F + 9.729(±2.291) R …(26)
(R = 0.915, n=10, P > 95%)

δAr-C-NH(ppm) = 137.65(±0.048) + 0.408(±0.104)σ_I + 0.233(±0.100)σ_R …(27)
(R = 0.986, n=10, P > 95%)

δAr-C-NH(ppm) =137.66(±0.042) + 0.404(±0.081)F + 0.237(±0.075) R …(28)
(R = 0.989, n=10, P > 95%)

δCS(ppm) = 110.58(±0.065) + 0.264(±0.140)σ_I + 0.600(±0.135)σ_R …(29)
(R = 0.987, n=10, P > 95%)

δCS(ppm) = 110.60(±0.067) + 0.232(±0.142)F + 0.524(±0.121) R …(30)
(R = 0.986, n=10, P > 95%)

δAr-C-N^+(ppm) = 135.71(±0.017) + 0.228(±0.036)σ_I + 0.293(±0.035)σ_R …(31)
(R = 0.996, n=10, P > 95%)

δAr-C-N^+(ppm) =135.72(±0.023) + 0.212(±0.048)F + 0.260(±0.041) R …(32)
(R = 0.993, n=10, P > 95%)

δCO_{syd}(ppm) = 174.66(±0.111) + 0.232(±0.023)σ_I + 0.559(±0.231)σ_R …(33)
(R = 0.970, n=10, P > 95%)

δCO_{syd}(ppm) =174.69(±0.107) + 0.169(±0.222)F + 0.509(±0.191) R …(34)
(R = 0.971, n=10, P > 95%)

δAr-C-CH_3(ppm) = 144.67(±0.032) + 0.186(±0.069)σ_I + 0.313(±0.067)σ_R …(35)
(R = 0.989, n=10, P > 95%)

δAr-C- CH_3(ppm) =144.69(±0.027) + 0.161(±0.057)F + 0.297(±0.049) R …(36)
(R = 0.992, n=10, P > 95%)

δCH_3(ppm) = 23.62(±0.640) +0.531(±0.137)σ_I +1.305(±0.137)σ_R …(37)
(R = 0.931, n=10, P > 90%)

δCH_3(ppm) = 23.44(±0.594) + 0.845(±0.125)F + 1.032(±0.106) R …(38)
(R = 0.942, n=10, P > 90%)

4. CONCLUSIONS

There are ten 4-(N-(4-(5-phenylisoxazol-3-yl)phenylsufamyl)-3-(p-tolyl)-1,2,3,-oxadiazol-3-ium-5-olates were prepared and examined their purities by literature method. The infrared and NMR spectral data of the synthesised sydnones were assigned and correlated with Hammett substituent constants and Swain-Lupton's constants using single and multi-regression analysis. From the results of statistical analyses, many single parameter correlations gave satisfactory correlation coefficients. All regression gave positive ρ values. This positive value inferred that the normal substituent effect operates in all systems.

The multi-regression analysis gave satisfactory correlation coefficients in all spectral data. In these correlations the probability factor was more than 90%. This implies that the degree of correlations was more than 90% feasible.

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